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SMALL HYPERFINE ANOMALY OF THE g-FACTOR RATIO OF FIRST-EXCITED AND GROUND STATES OF ^{129}I

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An unexpectedly small hyperfine anomaly $\epsilon = (-11 \pm 12) \times 10^{-4}$ is found between the 27.8 keV ($5/2^+$) and the ground state ($7/2^+$) of ^{129}I. A single-particle shell-model calculation yields a much larger anomaly, but mixing-in excited-state configurations reduces the calculated anomaly considerably.

The experimental fact that the ratio of the magnetic hyperfine splittings of a given pair of nuclear states differs from the ratio of the magnetic moments of those states is called the hyperfine anomaly. The effect is caused by the circumstance that, while magnetic moments are measured in a uniform external magnetic field, hyperfine splittings are caused by the slightly inhomogeneous hyperfine field of polarized atomic electrons (or muons). The distribution of nuclear magnetism over a finite volume then in principle leads to a small difference in the interaction energy ratio.

It can be shown by a classical argument [1] that the contact hyperfine interaction between the intrinsic spin of a nucleon and the spin of an atomic electron (s or $p_{1/2}$) at distance r from the centre of the nucleus is determined by the electronic charge density $|\psi_e(r)|^2$ while that of the orbital momentum of the nucleon is determined by the average of $|\psi_e(r)|^2$ within an orbital of radius r. For this reason, the absolute value of the spin part of the interaction is reduced more than the orbital part as a result of the finite nuclear size.

The hyperfine anomaly is observed by comparing h.f.s. splittings of pairs of nuclei in identical atomic electron environments. The effect has been observed both for pairs of ground states of different isotopes, generally by comparing NMR measurements of magnetic moments with atomic beam measurements of hyperfine splittings [2], and with the aid of Mössbauer spectroscopy, for the ground and isometric states of one isotope [3].

Large anomalies are expected – and have been found – for cases where a state with equal sign of orbital and spin contributions to the magnetic moment is compared with one where these contributions are of opposite sign. In such cases, an anomaly occurs even when the absolute values of the change of spin and orbital contributions are the same for both states. Perlow has reviewed [3] known cases where the hyperfine anomaly is particularly large for this reason. In some of the cases discussed by him, the anomalies were determined from Mössbauer spectra. Though the accuracy of the results of this method ($\approx 0.5\%$) is one or two orders of magnitude less than that of NMR + atomic beam measurements, the large value of the effect ($\approx 7\%$) rendered the method quite satisfactory for the cases studied.

In this paper we will treat a case where Mössbauer spectroscopy yields the anomaly with an accuracy of about 0.1%, and where the two states concerned have opposite spin–orbit coupling, so that a large

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hyperfine anomaly is expected.

The case in question is that of the 27.8 keV level ($5/2^+$) and ground state ($7/2^+$) of ^{129}I, between which a γ-transition of predominant M1 character, very suitable for Mössbauer spectroscopy, takes place. A long time ago the hyperfine splitting ratio $\Delta W^*/\Delta W$ of these states has been measured [4], using the magnetic hyperfine field experienced by ^{129}I impurities in ferromagnetic MnSb (0.007 ^{129m}Te). Due to the presence of a small admixture of quadrupole interaction, the Mössbauer spectrum is slightly asymmetric and this asymmetry turns out to be very sensitive to the hyperfine splitting ratio. This fact made it possible to determine this ratio quite accurately: $\Delta W^*/\Delta W = 1.0688(6)$ (this value was obtained from a reanalysis of the data used in ref. [4] by Reintsema [5]). The accuracy achieved here makes ^{129}I an interesting candidate for a hyperfine anomaly measurement. The magnetic moment ratio of the states considered had been determined for the first time from the Mössbauer spectrum of a K ^{129}I absorber placed in the external field of a 54 kG superconducting magnet, but the accuracy of this measurement was too small: $\mu^*/\mu = 1.078(20)$.

The recent completion of a Mössbauer spectrometer that can be operated in a 15 T Bitter Magnet of the High Magnetic Field Laboratory of the University of Nijmegen [6] provided a good opportunity to measure this magnetic moment ratio with better accuracy. In this spectrometer absorber and source are placed close together in the high-field region in order to get a sufficient count rate. Spectra were taken with a 20 mCi ^{129m}TeSn source and a ^{129}ICu absorber containing 5 mg ^{129}I/cm^2, yielding an effective thickness of $t_a = 5.4$. The source and the absorber experienced fields of 13.92 T and 13.86 T, respectively.

The zero-field spectrum, when fitted to a lorentzian line, yields a linewidth $\Gamma_{exp} = 1.22$ mm/s. This may be compared to a calculated value of 1.01 mm/s obtained with the formula

$$\Gamma_{exp} = 2(1.01 + 0.145 t_a - 0.0025 t_a^2)\Gamma_0,$$

valid for $t_a > 4$, assuming both source and absorber lines to have the natural width, Γ_0, at zero thickness. Since it is known that the absorber linewidth, Γ_a, extrapolates to Γ_0 for $t_a \to 0$ [7], we ascribe the excess width to the source. In a transmission integral fit of the zero-field spectrum we therefore started with a source linewidth $\Gamma_s = 0.50$ mm/s and fixed the absorber linewidth, Γ_a, at $\Gamma_0 = 0.294$ mm/s. This value for Γ_a was also inserted in the transmission integral fit of the high-field spectrum. In the fitting procedure the transmission integral function was calculated according to Cranshaw's method [8]. The variable fitting parameters for the zero-field spectrum were the source linewidth, Γ_s, the isomer shift, δ, and the fraction of recoilless γ-radiation, F. In the high-field spectrum, the variable parameters were δ, F, Γ_s, the gyromagnetic ratio of the ground state, g, and the magnetic moment ratio, μ^*/μ. Slightly lower χ^2 values for the fits of these two spectra were obtained by varying Γ_a as well. However, the values of the parameters in which we are interested do not change. The relative intensities of the $\Delta m = \pm 1$ transitions were chosen according to the appropriate Clebsch–Gordan coefficients, also taking into account the split-source spectrum. The intensities of the $\Delta m = 0$ lines were put equal to zero, because of the strong longitudinal field. The fits are shown as solid lines in fig. 1 and the parameter values are given in table 1.

The resulting hyperfine anomaly is

$$\epsilon = (\Delta W^*/\Delta W)/(\mu^*/\mu) - 1 = (-11 \pm 12) \times 10^{-4}. \quad (1)$$

In view of the qualitative arguments presented above, this value seems to be expectedly small. Let us see, however, what theoretical predictions can be made about the value of ϵ. The states involved have been assigned shell model character $d_{5/2}$ (27.8 keV) and $g_{7/2}$ (ground state). The $d_{5/2}$ and $g_{7/2}$ shells are filled in competition beyond the magic number $Z = 50$ and since iodine ($Z = 53$) has only three protons outside filled proton shells, we may first try the extreme single-particle model. For this model, Bohr and Weisskopf [9] (BW) have already given an expression in their pioneering paper about the hyperfine anomaly. In our particular case, this can be written as

$$\epsilon = -0.38 b \langle R^2/R_0^2\rangle g_s [(4g_l + g_s)^{-1} + (10 g_l - g_s)^{-1}]. \quad (2)$$

Taking $b = 0.013$ and $\langle R^2/R_0^2\rangle = 0.8$ according to BW, and $g_l = 1, g_s = 5.587$ for the odd proton, eq. (2) yields $\epsilon = -0.0073$. In their paper BW neglected a term that takes into account the angular asymmetry of the electron–nuclear interaction. If this term is added

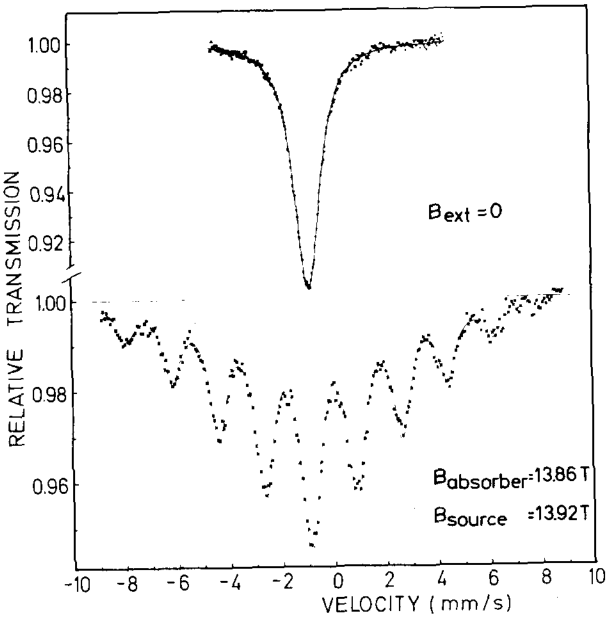

Fig. 1. ^{129}I Mössbauer spectrum of ^{129}ICu at zero field and in a high external field (B_{source} = 13.92 T, $B_{absorber}$ = 13.86 T). The solid line represents a transmission integral fit to the measured data.

explicitly to the expression of BW, as done by Perlow [3], the calculated anomaly increases to $\epsilon = -0.0184$. A more refined theoretical treatment was presented by Stroke, Blin-Steyle and Jaccarino [2] (to be indicated as SBJ). They also incorporated the asymmetry term in their treatment but at the same time found considerably reduced values for the parameters equivalent to b and $\langle R^2/R_0^2\rangle$ in eq. (2). In the single-particle limit of their theory, a value $\epsilon =$ -0.0069 results.

Thus, all single-particle estimates of ϵ turn out to be much larger than the experimental result.

In itself, this is not surprising, since the magnetic moments themselves, $\mu^* = 2.797$ n.m. and $\mu = 2.617$ n.m., deviate considerably from the single-particle (Schmidt) values $\mu^*_{sp} = 4.792$ n.m. and $\mu_{sp} = 1.718$ n.m. The main feature of the SBJ treatment, however, is the addition of terms that represent the mixing of core-excited configurations into the single-particle shell model states. As had been shown earlier by Blin-Stoyle [10] and by Arima and Horie [11] this leads to much better magnetic moment values in a number of cases. Table 1 shows that this is also true for our case. The table gives the magnetic moment values calculated from the formulas and coefficients given by SBJ for the seniority 1 proton configurations $(2d_{5/2})(1g_{7/2})$ and $(d_{5/2})^3$ of the $5/2^+$ state and the $(1g_{7/2})(2d_{5/2})$ and $(1g_{7/2})^3$ configurations of the $7/2^+$ state, choosing an outer-shell neutron configuration $(h_{11/2})^{12}(d_{5/2})^6$ in each case. The excited-state admixtures included in the calculation are also given in the table. The agreement with experiment is clearly improved, especially for the proton configurations $(2d_{5/2})^3$ and $(1g_{7/2})(2d_{5/2})^2$. The closeness in energy of the $2d_{5/2}$ and $1g_{7/2}$ states in this region, however, undoubtedly leads to mixed zero-order configurations for both states considered.

Also, the effect of the higher-seniority state $(g_{7/2})^3$ ($J = 5/2$) should certainly be taken into account, because it is expected to lie close to the $7/2^+$ ground state. By SBJ, however, no explicit expressions are given for such mixed configurations.

Therefore we could only take into account the zero-order and excited configurations given in table 2 and the $d_{5/2} \to g_{7/2}$ ($l = 2$) proton excitation in the calculation of the hyperfine anomalies with the aid of SBJ's formulas and tabulated coefficients. The values thus obtained are given in table 3. They are reduced to about one half of the single-particle value, but they are still larger than the experimental value. The same mechanism that causes the magnetic moments to deviate from their Schmidt values apparently also serves to reduce the hyperfine anomaly.

As shown by SBJ the configurational mixing cor-

Table 1
Final values of fixed and adjustable parameters obtained with a transmission integral fit procedure.

B_{source} (T)	B_{abs} (T)	δ (mm/s)	F	Γ_a (mm/s)	Γ_s (mm/s)	t_a	g (mm/s/T)	μ^*/μ
13.92	13.86	−0.838(2)	0.152(5)	0.294	0.504(2)	5.45	0.2545(3)	1.070(1)
0	0	−0.841(2)	0.161(5)	0.294	0.500(2)	5.45	–	–

Table 2
Values of magnetic moments of $5/2^+$ (27.8 keV) and $7/2^+$ (ground) states of ^{129}I, calculated from Stroke et al. [2], compared with single-particle and experimental values.

State	Zero-order proton configurations	Excited configurations: protons	Excited configurations: neutrons	μ_{calc} (n.m.)	μ_{sp} (n.m.)	μ_{exp} (n.m.)
$5/2^+$	$(2d_{5/2})(1g_{7/2})^2$	$g_{9/2} \to g_{7/2}$	$h_{11/2} \to g_{9/2}$ $d_{5/2} \to d_{3/2}$	3.657	4.792	2.797
	$(2d_{5/2})^3$	$g_{9/2} \to g_{7/2}$ $d_{5/2} \to d_{3/2}$	$h_{11/2} \to h_{9/2}$ $d_{5/2} \to d_{3/2}$	3.026		
$7/2^+$	$(1g_{7/2})(2d_{5/2})^2$	$g_{9/2} \to g_{7/2}$ $d_{5/2} \to d_{3/2}$	$h_{11/2} \to h_{9/2}$ $d_{5/2} \to d_{3/2}$	2.762	1.781	2.617
	$(1g_{7/2})^3$	$g_{9/2} \to g_{7/2}$	$h_{11/2} \to h_{9/2}$ $d_{5/2} \to d_{3/2}$	2.229		

Table 3
Values of hyperfine anomalies ϵ for zero-order proton configurations listed in table 2, calculated using formulas of Stroke et al. [2].

		27.8 keV state: $(d_{5/2})(g_{7/2})^2$	27.8 keV state: $(d_{5/2})^3$
ground state	$(g_{7/2})(d_{5/2})^2$	−0.0035	−0.0032
	$(g_{7/2})^3$	−0.0042	−0.0039

rections both to the magnetic moments and to the hyperfine anomaly coefficients of each of the nuclear states concerned, are proportional to coefficients α, which, in turn are proportional to the singlet interaction energy V_s between nucleons. By increasing V_s above the value chosen by SBJ we can increase the configurational mixing correction to the extent that the calculated moments coincide with the measured moments. If we do this, we obtain adjusted values for the coefficients α, with which we can recalculate the hyperfine anomaly. It turns out, that somewhat smaller values, $\epsilon = -0.0025$ to -0.0030, are thus obtained. They are still larger than the experimental result, but not much outside our limits of error.

In conclusion we may say that configurational mixing leads to a considerable reduction of the hyperfine anomaly for ^{129}I and thus goes a long way towards explaining the small value measured.

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